Structure and Bonding in WC_n (n = 2-5) clusters

Supplementary material

Theoretical Chemistry Accounts

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Content: Tables 1SI-3SI; Cartesian coordinates for all structures reported in the paper at PBE0/def2-TZVP level of theory; Cartesian coordinates for the global minima, reoptimized using the B3LYP/def2-TZVP model chemistry; and Cartesian coordinates for the first 2 most stable WC_2 structures (quintuplet and triplet) reoptimized at CCSD/def2-TZVP level of theory.

Tables 1SI, 2SI, 3SI

Table 1SI. Energies (kcal mol^{-1}) and Boltzmann populations for WC_3 clusters.[a]

structure	-AE	ΔAE= ΔE	ΔG	%pop$_{\Delta E}$	%pop$_{\Delta G}$	ΔE$_{SR}$	ΔE$_{SO}$
$^3S_1$	-435.61	0.00	0.00	71.36	68.00	6.20	5.99
$^3S_2$	-435.07	0.54	0.45	28.59	31.98	0.00	0.00
$^1S_3$	-431.23	4.28	5.09	0.05	0.01	6.73	0.71
$^5S_4$	-422.24	13.34	12.95	0.00	0.00	14.50	13.99
$^5S_5$	-418.32	17.38	16.85	0.00	0.00	17.73	8.00
$^3S_6$	-408.62	26.98	26.96	0.00	0.00	27.22	20.30
$^1S_7$	-400.79	34.86	35.38	0.00	0.00	34.25	34.04
$^3S_8$	-393.41	42.21	41.88	0.00	0.00	40.24	39.31

[a] -AE: Negative values of ZPE-corrected atomization energies. ΔAE: Relative ZPE-corrected atomization energies (relative ZPE-corrected energies, ΔE). ΔG: Relative Gibbs free energies. %**pop**$_{\Delta E}$, %**pop**$_{\Delta G}$: Boltzmann populations at standard conditions based on the relative ZPE-corrected energies and on the relative Gibbs free energies, respectively. These values are based on calculations at PBE0/def2-TZVP level. Δ**E**$_{SR}$ and Δ**E**$_{SO}$ are the ZORA relative energies at scalar relativistic and spin-orbit (2 components) approximations, respectively. They were calculated using the all-electron PBE0/TZ2P model chemistry over the PBE0/def2-TZVP geometries.

Table 2SI. Energies (kcal mol^{-1}) and Boltzmann populations for WC_4 clusters.[a]

structure	-AE	ΔAE= ΔE	ΔG	%pop$_{\Delta E}$	%pop$_{\Delta G}$	ΔE$_{SR}$	ΔE$_{SO}$
$^3S_1$	-587.58	0.00	0.00	100.00	100.00	0.00	0.00
$^1S_2$	-581.13	6.50	7.01	0.00	0.00	6.21	0.40
$^3S_3$	-578.59	8.95	9.02	0.00	0.00	9.43	10.42
$^5S_4$	-575.36	12.16	11.59	0.00	0.00	12.52	11.54
$^5S_5$	-563.14	24.43	23.88	0.00	0.00	33.47	33.15
$^1S_6$	-559.68	27.89	28.34	0.00	0.00	27.92	11.56
$^3S_7$	-557.04	30.56	29.64	0.00	0.00	30.35	31.27
$^5S_8$	-555.85	31.75	30.86	0.00	0.00	32.16	32.60

[a] -AE: Negative values of ZPE-corrected atomization energies. ΔAE: Relative ZPE-corrected atomization energies (relative ZPE-corrected energies, ΔE). ΔG: Relative Gibbs free energies. %**pop**$_{\Delta E}$, %**pop**$_{\Delta G}$: Boltzmann populations at standard conditions based on the relative ZPE-corrected energies and on the relative Gibbs free energies, respectively. These values are based on calculations at PBE0/def2-TZVP

level. ΔE_{SR} and ΔE_{SO} are the ZORA relative energies at scalar relativistic and spin-orbit (2 components) approximations, respectively. They were calculated using the all-electron PBE0/TZ2P model chemistry over the PBE0/def2-TZVP geometries.

Table 3SI. Energies (kcal mol^{-1}) and Boltzmann populations for WC_4 clusters.[a]

structure	-AE	$\Delta AE = \Delta E$	ΔG	$\%pop_{\Delta E}$	$\%pop_{\Delta G}$	ΔE_{SR}	ΔE_{SO}
$^3S_1$	-727.56	0.00	0.00	99.36	99.19	0.00	0.00
$^3S_2$	-724.56	3.06	2.91	0.60	0.78	2.97	4.41
$^3S_3$	-722.81	4.76	4.84	0.03	0.03	4.80	5.36
$^3S_4$	-716.45	11.12	11.15	0.00	0.00	10.80	12.60
$^1S_5$	-715.34	12.19	12.67	0.00	0.00	12.07	11.11
$^1S_6$	-714.88	12.82	13.68	0.00	0.00	12.58	5.95
$^5S_7$	-714.19	13.34	12.80	0.00	0.00	13.61	10.49
$^5S_8$	-711.33	16.24	15.28	0.00	0.00	16.32	16.09

[a] -AE: Negative values of ZPE-corrected atomization energies. ΔAE: Relative ZPE-corrected atomization energies (relative ZPE-corrected energies, ΔE). ΔG: Relative Gibbs free energies. $\%pop_{\Delta E}$, $\%pop_{\Delta G}$: Boltzmann populations at standard conditions based on the relative ZPE-corrected energies and on the relative Gibbs free energies, respectively. These values are based on calculations at PBE0/def2-TZVP level. ΔE_{SR} and ΔE_{SO} are the ZORA relative energies at scalar relativistic and spin-orbit (2 components) approximations, respectively. They were calculated using the all-electron PBE0/TZ2P model chemistry over the PBE0/def2-TZVP geometries.

Cartesian coordinates for all structures reported in the paper at PBE0/def2-TZVP level of theory

----------WC_2----------

$^5S_1$

C	0.652838	-1.614461	0.000000
C	-0.652838	-1.614346	0.000000
W	0.000000	0.261795	0.000000

$^3S_2$

C	0.718160	-1.472091	0.000000
C	-0.718160	-1.472090	0.000000
W	0.000000	0.238717	0.000000

$^5S_3$

C	0.620609	-1.853508	0.000000
C	-0.620609	-1.522994	0.000000
W	0.000000	0.273770	0.000000

$^5S_4$

C	0.000544	-2.815321	0.000000
C	-0.000544	-1.525521	0.000000
W	0.000000	0.351960	0.000000

$^1S_5$

C	0.781159	-1.384731	0.000000
C	-0.781159	-1.385280	0.000000
W	0.000000	0.224596	0.000000

$^3S_6$

C	0.001110	-2.797187	0.000000
C	-0.001110	-1.493429	0.000000
W	0.000000	0.347888	0.000000

$^3S_7$

C	1.059129	-1.207543	0.000000
C	-1.059129	-1.207464	0.000000
W	0.000000	0.195811	0.000000

$^5S_8$

W	0.000000	0.155716	0.000000
C	1.439527	-1.066112	0.000000
C	-1.439527	-0.854385	0.000000

----------WC_3----------

$^3S_1$

C	1.150410	-1.221684	0.000143
C	1.683795	0.000661	-0.000210
C	1.148165	1.222647	0.000143
W	-0.322895	-0.000132	-0.000006

$^3S_2$

W	0.308254	-0.000039	0.000032
C	-1.073347	-1.271105	-0.000659
C	-1.655692	0.000127	0.000928
C	-1.072764	1.271461	-0.000659

$^1S_3$

C	1.639662	0.000039	-0.000099
C	1.102861	-1.228707	0.000068
C	1.102736	1.228761	0.000068
W	-0.311778	-0.000008	-0.000003

$^{5}S_{4}$

C	1.425300	0.722810	0.000319
C	2.630829	-0.000366	-0.000389
C	1.425655	-0.722071	0.000320
W	-0.444469	-0.000030	-0.000020

$^{5}S_{5}$

C	-1.277903	1.259243	-0.039619
C	-1.729009	0.000742	0.062078
C	-1.280603	-1.258102	-0.039621
W	0.347636	-0.000153	0.001391

$^{3}S_{6}$

W	0.417708	-0.000057	-0.000002
C	-2.520790	0.000112	-0.000038
C	-1.314559	0.746625	0.000032
C	-1.316382	-0.746029	0.000032

$^{1}S_{7}$

C	-1.239002	-0.843139	-0.504101
C	-1.239553	0.858214	-0.477652
C	-1.239237	-0.015380	0.981774
W	0.301443	0.000025	-0.000002

$^{3}S_{8}$

C	-1.600902	0.349683	-0.657667
C	1.089702	1.349764	-0.000328
C	-1.599673	0.350214	0.657953
W	0.171152	-0.166189	0.000003

$^{1}S_{9}$

C	1.292949	0.766892	0.142467
C	1.292408	-0.766551	0.142608
C	2.451171	-0.000348	-0.169582
W	-0.408367	0.000001	-0.009364

$^{1}S_{3}$

C	1.669449	0.770081	-0.391389
C	-1.017819	1.325400	0.252275
C	1.677506	-0.178060	0.501751
W	-0.188849	-0.155467	-0.029403

$^{1}S_{11}$

C	1.018328	1.324789	0.252368
C	-1.669349	0.770737	-0.390852
C	-1.678621	-0.178517	0.500998
W	0.188890	-0.155433	-0.029393

$^{1}S_{12}$

C	-1.007788	1.378218	-0.000100
C	1.570886	0.242839	0.000811
C	2.855728	0.178146	-0.000502
W	-0.277202	-0.145881	-0.000017

$^{5}S_{13}$

C	1.166803	1.340068	0.214539
C	-1.810293	-0.121987	0.371977
C	-1.512672	0.931248	-0.311467
W	0.174824	-0.174270	-0.022301

$^{5}S_{14}$

C	1.512356	0.931630	-0.311687
C	1.809673	-0.121144	0.372476
C	-1.168433	1.339530	0.214620
W	-0.174616	-0.174326	-0.022330

$^{5}S_{15}$

C	1.901851	0.609007	0.000037
C	-2.105692	-0.183430	0.000045
C	-1.462631	0.930674	-0.000022
W	0.135119	-0.109966	-0.000005

$^{5}S_{16}$

C	-0.741361	1.557556	-0.000144
C	1.581106	0.266597	0.000858
C	2.853376	0.059301	-0.000532
W	-0.299442	-0.152712	-0.000015

----------WC_4----------

$^{3}S_{1}$

C	-1.502763	0.698706	0.000100
C	-0.684612	1.764616	0.000093
C	-0.730641	-1.746581	0.000245
C	-1.520562	-0.659358	-0.000293
W	0.359885	-0.004653	-0.000012

$^{1}S_{2}$

C	1.758788	0.676230	0.000093
C	0.685042	1.481777	-0.000011
C	-0.678550	1.485154	-0.000116
C	-1.755462	0.683648	0.000134
W	-0.000796	-0.350822	-0.000008

$^{3}S_{3}$

C	2.523958	-0.334289	-0.002472
C	1.458550	0.621098	0.003326
C	0.428557	1.573634	-0.001182
C	1.262143	-0.924636	0.001187

W	-0.459990	-0.075876	-0.000070

$^{5}S_{4}$

C	0.869955	1.728380	0.000328
C	1.616158	0.688786	-0.000273
C	1.617371	-0.687152	-0.000096
C	0.872005	-1.727535	0.000257
W	-0.403418	-0.000201	-0.000018

$^{5}S_{5}$

C	-2.165077	-0.574545	-0.000379
C	-1.651769	0.750526	-0.000327
C	-0.721548	1.615748	0.000546
C	-1.075592	-1.291613	0.000678
W	0.455188	-0.040550	-0.000042

$^{1}S_{6}$

C	1.243312	-0.952184	0.000594
C	1.410427	0.668901	0.000375
C	2.478787	-0.333734	-0.000596
C	0.394499	1.595221	0.000051
W	-0.448137	-0.079314	-0.000034

$^{3}S_{7}$

W	0.657476	-0.099905	-0.000006
C	-2.600584	-0.022733	0.000355
C	-1.331584	0.347245	0.000161
C	-0.383657	1.365687	-0.000141
C	-3.793044	-0.458034	-0.000299

$^{5}S_{8}$

W	0.457840	-0.000100	0.000003
C	-0.843163	-1.397002	-0.000073
C	-0.842290	1.397723	-0.000011
C	-1.981282	-0.724364	0.000082
C	-1.979953	0.724874	-0.000038

$^{1}S_{9}$

C	-0.852228	1.505747	-0.000041
C	2.645902	0.122689	-0.000080
C	1.446190	0.093001	-0.713620
C	1.446350	0.093105	0.713680
W	-0.379963	-0.147125	0.000005

$^{3}S_{10}$

C	1.822001	0.200031	0.522261
C	-1.412872	1.035236	0.406229
C	-2.138713	0.217703	-0.251894
C	1.701084	0.922525	-0.538493
W	0.002311	-0.192608	-0.011198

$^{3}S_{11}$

C	1.822171	0.199196	0.521926
C	-1.413526	1.034849	0.406512
C	1.700832	0.922655	-0.538152
C	-2.138414	0.216935	-0.252152
W	0.002346	-0.192457	-0.011200

$^{3}S_{12}$

C	2.138518	0.217790	-0.252306
C	-1.699981	0.923250	-0.538127
C	1.412802	1.034592	0.407033
C	-1.822403	0.199455	0.521633
W	-0.002346	-0.192575	-0.011208

$^{1}S_{13}$

C	-1.468679	0.923970	-0.502350
C	2.025947	0.143387	-0.365599
C	1.469213	0.922607	0.503813
C	-2.027164	0.142498	0.363718
W	0.000055	-0.172902	0.000034

$^{1}S_{14}$

C	-2.026410	0.143553	-0.364798
C	1.468362	0.923910	-0.502819
C	-1.468563	0.923460	0.503278
C	2.026715	0.143288	0.364227
W	-0.000008	-0.173044	0.000009

$^{1}S_{15}$

W	-0.000001	0.173012	0.000001
C	1.468473	-0.923748	-0.502904
C	-2.026533	-0.143299	-0.364567
C	2.026610	-0.143196	0.364387
C	-1.468535	-0.923576	0.503069

$^{1}S_{16}$

C	1.622306	0.703880	-0.641381
C	1.622229	0.702502	0.642345
C	-1.621830	0.702605	0.642345
C	-1.622090	0.704131	-0.641308
W	-0.000050	-0.228091	-0.000162

$^{1}S_{17}$

C	0.959827	0.005941	1.463766
C	-1.287410	-1.218942	0.141177
C	-1.770891	0.000772	0.281152
C	-1.288172	1.219942	0.132720
W	0.274593	-0.000625	-0.163688

$^{1}S_{18}$

C	1.645203	0.521483	0.600790
C	-1.658953	0.261884	0.583774
C	-1.696664	1.279459	-0.214415
C	1.316262	1.411850	-0.274665
W	0.031958	-0.281730	-0.056391

$^{5}S_{19}$

W	-0.773416	-0.000003	-0.000001
C	1.156124	0.000150	-0.000004
C	2.388588	-0.737890	0.000035
C	2.389114	0.738021	0.000034
C	3.604965	-0.000249	-0.000048

$^{3}S_{20}$

C	1.660350	0.251193	0.578513
C	1.711168	1.275748	-0.210252
C	-1.640823	0.537352	0.601634
C	-1.298366	1.417505	-0.278965
W	-0.035054	-0.282308	-0.056021

$^{1}S_{21}$

C	1.755753	-0.048785	0.000567
C	1.633339	1.259571	-0.000253
C	-0.964500	1.250091	0.689975
C	-0.964006	1.250469	-0.689645
W	-0.118426	-0.300920	-0.000052

$^{3}S_{22}$

C	1.203257	0.869985	1.029694
C	-1.405321	-0.910724	0.660824
C	-1.079355	1.316773	-0.423842
C	-1.713245	0.304477	0.235285
W	0.242811	-0.128150	-0.121781

$^{3}S_{23}$

W	0.388277	-0.149096	-0.000042
C	0.816530	1.540283	0.000452
C	-1.469835	0.105984	-0.723578
C	-1.470041	0.104904	0.723707
C	-2.665404	0.087683	-0.000064

$^{5}S_{24}$

C	1.739487	0.670157	0.562269
C	-1.870326	0.660019	0.509361
C	-1.870540	-0.623670	0.552687
C	1.740220	-0.629953	0.606633
W	0.021175	-0.006207	-0.180888

$^{1}S_{25}$

W	-0.580686	-0.127781	-0.000059
C	1.269503	-0.016400	0.000811
C	-0.531696	1.597633	-0.000082
C	2.576026	0.019340	0.001160
C	3.847962	-0.024607	-0.001165

$^{5}S_{26}$

C	1.984465	0.236123	0.004372
C	1.323080	1.335665	-0.002346
C	-1.321713	1.336227	0.000160
C	-1.983989	0.236963	0.002702
W	-0.000149	-0.254998	-0.000396

$^{3}S_{27}$

W	0.585917	-0.028588	0.000002
C	-2.262406	0.628420	0.000127
C	-0.960575	1.012509	-0.000106
C	-2.732714	-0.659280	-0.000084
C	-1.270620	-0.629060	0.000043

$^{5}S_{28}$

C	-2.080895	0.127385	-0.259168
C	1.495400	1.166218	-0.434257
C	1.889825	0.250847	0.385296
C	-1.644198	1.142741	0.374783
W	0.027557	-0.217880	-0.005404

$^{3}S_{29}$

C	-1.282753	-1.193304	0.000012
C	-1.451231	0.000022	0.793963
C	-1.282759	1.193307	-0.000021
C	-1.451282	-0.000029	-0.793934
W	0.443353	0.000000	-0.000002

$^{3}S_{30}$

W	0.411175	-0.000021	-0.009699
C	-1.176972	-0.003747	1.090138
C	-1.117972	-1.258635	-0.258798
C	-1.117057	1.260835	-0.254454
C	-1.659156	0.001807	-0.457267

$^{5}S_{31}$

C	1.536224	0.838872	0.680103
C	-1.828743	0.312311	0.024955
C	-3.000300	0.696298	-0.011141
C	1.724785	1.005497	-0.591093
W	0.127138	-0.231322	-0.008337

$^{3}S_{32}$

W	-0.389914	-0.033953	0.000000
C	0.673827	1.506715	-0.000012
C	1.242079	-0.755298	0.794338
C	1.650950	0.422633	0.000018
C	1.242086	-0.755300	-0.794349

$^{5}S_{33}$

W	0.464692	0.000310	0.000200
C	-1.300938	-1.228496	-0.117777
C	-1.565028	-0.193794	0.757691
C	-1.307528	1.224331	0.123141
C	-1.557712	0.194141	-0.765516

$^{3}S_{34}$

W	-0.464123	0.000000	-0.000002
C	1.574494	-0.001054	0.864189
C	1.287574	-1.135214	-0.000786
C	1.574538	0.001049	-0.864194
C	1.287577	1.135218	0.000814

$^{1}S_{35}$

W	-0.374546	-0.000286	0.000567
C	1.006615	-0.191164	1.284934
C	1.620793	0.002680	-0.005426
C	0.993990	1.213950	-0.478143
C	0.998004	-1.021933	-0.808361

$^{3}S_{36}$

C	-2.396805	-0.001158	0.037483
C	-1.213039	0.849881	-0.468906
C	-1.213765	-0.841746	-0.479544
C	-1.221658	-0.005784	0.880663
W	0.490157	-0.000097	0.002457

$^{3}S_{37}$

W	-0.430410	-0.000031	-0.000366
C	1.218666	1.207972	-0.002974
C	1.441086	0.000258	-0.830217
C	1.219231	-1.207789	-0.003190
C	1.429405	-0.000055	0.840899

$^{5}S_{38}$

W	-0.178267	0.000288	-0.087504
C	1.283205	1.226729	0.164051
C	-2.167406	-0.001078	0.495551
C	1.281570	-1.228157	0.162955
C	1.801264	-0.001043	0.256665

$^{5}S_{39}$

C	-1.402102	0.795830	-0.001740
C	-1.853280	-0.605885	0.002043
C	1.527013	1.199987	0.001819
C	-2.720709	0.434223	0.000216
W	0.360736	-0.147904	-0.000190

$^{5}S_{40}$

C	-1.205813	0.002726	1.342844
C	1.313690	1.237478	0.209609
C	1.314906	-1.236177	0.213685
C	1.829098	0.000966	0.285370
W	-0.263666	-0.000405	-0.166338

$^{5}S_{41}$

C	-1.352631	-0.203593	0.003035
C	-2.622217	0.016282	0.003960
C	-3.914123	0.163510	-0.004096
C	0.817762	1.610592	0.000489
W	0.573341	-0.128659	-0.000275

$^{5}S_{42}$

W	0.517581	-0.032509	-0.000200
C	-2.379047	-0.616772	-0.003653
C	-1.375631	-0.058283	-0.860132
C	-1.253354	1.146576	0.007126
C	-1.375470	-0.070578	0.859128

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$^{3}S_{1}$

C	-1.158837	1.299730	0.136486
C	-1.826949	0.242324	0.503761
C	1.154953	1.303270	0.137002
C	1.825583	0.247038	0.503651
C	-0.002490	1.723386	-0.521601
W	0.000628	-0.390466	-0.061565

$^{3}S_{2}$

C	-2.785162	-0.000334	-0.001150
C	-1.816516	0.925229	0.000003
C	-0.622535	-1.445099	0.001339
C	-1.817279	-0.925521	0.000181
C	-0.623084	1.446513	0.001451
W	0.621452	-0.000064	-0.000148

$^{3}S_{3}$

W	-0.490776	0.000005	-0.064340
C	0.416876	-1.581533	0.570531
C	2.321186	-0.000065	-0.414639
C	0.416984	1.581573	0.570489

C	1.448957	0.946847	0.033583
C	1.448898	-0.946889	0.033560

$^{3}S_{4}$

W	0.693331	0.000051	-0.000029
C	-2.181259	-1.288619	0.000264
C	-2.466527	-0.000306	-0.000126
C	-2.182148	1.288446	-0.000536
C	-0.860316	-1.061104	-0.000106
C	-0.860832	1.060957	0.000865

$^{1}S_{5}$

C	-2.673602	0.000174	-0.197034
C	-1.643292	0.855354	-0.023278
C	-0.528552	-1.464278	0.338352
C	-1.643650	-0.855396	-0.023504
C	-0.528242	1.464541	0.338173
W	0.568973	-0.000032	-0.035085

$^{1}S_{6}$

C	1.327097	-1.044023	0.128047
C	0.286927	-1.696706	0.617679
C	1.323121	1.047740	0.127264
C	0.281504	1.697369	0.618201
C	1.959400	0.002694	-0.552964
W	-0.419842	-0.000574	-0.076072

$^{5}S_{7}$

C	1.225312	1.308218	0.033785
C	-1.901772	0.324404	0.548012
C	0.001536	1.711489	-0.431483
C	1.902471	0.321553	0.548168
C	-1.222859	1.310287	0.034095
W	-0.000380	-0.403455	-0.059398

$^{5}S_{8}$

W	0.439267	-0.002562	-0.000021
C	-1.341676	-1.117004	0.000006
C	-2.122234	0.012646	-0.000116
C	-1.327174	1.132373	0.000012
C	-0.301371	1.936173	0.000174
C	-0.325171	-1.932589	0.000178

$^{1}S_{9}$

C	-2.042305	-0.091147	0.385042
C	-0.297359	1.525084	-0.381960
C	0.952190	1.420665	0.188521
C	1.856014	0.460516	0.308932
C	-1.530771	1.023316	0.022874
W	0.086127	-0.351765	-0.042439

$^{5}S_{10}$

C	0.138500	1.895689	0.000233
C	-1.053631	1.446042	0.000133
C	-1.355267	-0.916754	0.000271
C	-2.744015	-0.726521	0.000227
C	-1.930556	0.408468	-0.000635
W	0.563106	-0.170832	-0.000019

$^{3}S_{11}$

C	0.075376	1.853817	0.000284
C	-2.603781	-0.808377	-0.000231
C	-1.101429	1.363751	-0.000035
C	-1.141110	-0.930560	0.000711
C	-2.043859	0.380274	-0.000213
W	0.552552	-0.150722	-0.000042

$^{5}S_{12}$

W	-0.581467	-0.000069	-0.012486
C	1.680173	-0.992876	-0.013558
C	0.598798	-1.660629	0.128314
C	2.615278	0.000602	-0.075584
C	1.679430	0.993127	-0.013457
C	0.597743	1.660626	0.128277

$^{1}S_{13}$

C	-1.346553	1.233847	0.298021
C	-1.839315	0.000719	0.442402
C	-1.347319	-1.232849	0.299474
C	1.558483	0.000631	1.087786
C	2.237498	0.000403	0.023138
W	0.059773	-0.000223	-0.174391

$^{5}S_{14}$

W	-0.600364	-0.262419	0.000000
C	-0.784502	1.754968	0.000142
C	3.747560	-0.529661	0.000317
C	1.344459	0.463297	-0.000016
C	2.590868	0.005929	-0.000399
C	0.506103	1.541962	-0.000046

$^{1}S_{15}$

C	1.300526	-1.242796	0.436732
C	-1.727847	0.650867	0.715995
C	-1.727877	-0.649789	0.716748
C	1.743040	0.000579	0.647561
C	1.300296	1.243526	0.435487
W	-0.072011	-0.000194	-0.239394

$^{3}S_{16}$

C	1.027735	1.558813	0.002621
C	-1.266903	0.500797	-0.002627
C	-2.537462	0.087336	-0.003857
C	-0.337307	1.522282	-0.000410
C	-3.697151	-0.422139	0.004308
W	0.552250	-0.263278	-0.000003

$^{3}S_{17}$

C	-1.473671	1.231073	0.282071
C	-1.886204	0.000865	0.548697
C	1.863152	-0.637981	0.555689
C	1.863398	0.638383	0.553629
C	-1.475841	-1.229902	0.282195
W	0.089932	-0.000198	-0.180185

$^{5}S_{18}$

C	-0.877395	-1.251857	-0.035066
C	-2.192290	-1.068022	-0.062312
C	-0.363825	1.649674	-0.080645
C	-2.553959	0.259159	0.094856
C	-1.533371	1.133073	0.002413
W	0.609798	-0.058543	0.006548

$^{3}S_{19}$

C	2.798782	0.541450	0.000170
C	1.609160	0.277314	0.712214
C	-1.794433	0.821843	0.641247
C	1.608758	0.279655	-0.711681
C	-1.795459	0.822324	-0.639737
W	-0.196768	-0.222372	-0.000179

$^{1}S_{20}$

C	1.144618	-0.886919	0.025147
C	2.628625	-0.735320	0.036637
C	-0.173806	1.809036	0.063072
C	2.049941	0.435028	-0.047101
C	1.008706	1.314141	-0.038454
W	-0.539845	-0.156970	-0.003187

$^{3}S_{21}$

C	2.042767	0.003123	0.135611
C	-1.392461	-1.215900	0.352935
C	-1.390047	1.228947	0.311097
C	1.487698	0.022518	1.300547
C	-1.837006	0.011044	0.572639
W	0.088301	-0.004032	-0.216716

$^{1}S_{22}$

C	2.686163	0.549459	-0.000462

C	1.510772	0.295549	0.732313
C	-1.424356	1.104136	0.669176
C	1.510468	0.296001	-0.731816
C	-1.425005	1.103800	-0.669028
W	-0.231733	-0.271536	-0.000015

$^{1}S_{23}$

C	-1.441691	0.216719	0.912485
C	0.428960	1.582201	-0.000491
C	-0.993197	1.290881	-0.000295
C	1.656307	1.129974	0.000248
C	-1.442076	0.215912	-0.911903
W	0.145273	-0.359650	-0.000004

$^{3}S_{24}$

W	0.039200	-0.274920	0.028580
C	1.660488	0.962253	-0.093691
C	-1.737805	0.429338	-0.079849
C	1.274019	0.754521	1.158660
C	1.302488	0.474206	-1.274815
C	-2.982662	0.770355	-0.062786

$^{1}S_{25}$

W	-0.364958	-0.000289	-0.149098
C	-1.197050	0.001515	1.329732
C	1.842460	0.685197	0.243547
C	1.007143	-1.593460	0.011206
C	1.842999	-0.683665	0.244580
C	1.005598	1.593978	0.009814

$^{3}S_{26}$

C	-1.665142	0.672886	0.292583
C	-1.665366	-0.672535	0.292278
C	-0.898529	-1.692561	0.040140
C	1.233292	-0.001226	1.369879
C	-0.897396	1.692766	0.041011
W	0.315660	0.000054	-0.165072

$^{3}S_{27}$

W	0.651800	-0.097674	-0.000007
C	-0.205134	1.695405	-0.000007
C	-1.255043	0.945801	0.000065
C	-2.166349	-0.155489	0.000026
C	-3.474880	-0.308265	-0.000077
C	-0.937463	-0.972805	0.000080

$^{3}S_{28}$

C	-1.597471	0.775761	0.734476
C	1.806552	-0.305218	0.441133
C	-2.280568	0.703657	-0.351215

C	1.463839	0.830267	-0.348472
C	2.795906	0.613575	0.000360
W	-0.177426	-0.212274	-0.038617

$^{3}S_{29}$

W	-0.465375	-0.264121	0.000013
C	-1.129473	1.425254	-0.661395
C	2.667568	0.160153	-0.000271
C	1.396020	-0.120702	-0.000069
C	-1.129905	1.425432	0.661297
C	3.935416	0.367360	0.000272

$^{5}S_{30}$

W	0.679451	0.000014	-0.000002
C	-2.287154	1.439240	-0.000003
C	-1.852956	0.000073	0.000091
C	-2.287018	-1.439282	-0.000084
C	-0.976413	1.192669	-0.000041
C	-0.976353	-1.192866	0.000056

$^{3}S_{31}$

C	0.872210	-1.110239	-0.980216
C	1.415349	1.062117	-0.000893
C	1.621831	-0.339901	-0.000405
C	0.432277	1.890360	0.000241
C	0.872767	-1.108385	0.981542
W	-0.422792	-0.031942	-0.000022

$^{1}S_{32}$

C	-0.429235	1.482719	-0.643818
C	-1.579982	-0.743710	-0.198946
C	-1.434686	-0.000666	1.026664
C	-1.580564	0.742560	-0.199327
C	-0.427439	-1.482168	-0.644509
W	0.442046	0.000103	0.053508

$^{1}S_{33}$

W	-0.654553	-0.082899	-0.000001
C	0.197662	1.622725	-0.000071
C	2.225086	-0.270326	0.000063
C	3.521693	-0.097730	-0.000067
C	0.943818	-0.958701	-0.000039
C	1.184556	0.726459	0.000121

$^{5}S_{34}$

C	1.505953	1.250341	-0.234232
C	1.971127	0.207364	0.446933
C	1.465508	-0.946156	0.871541
C	-2.036510	-0.034728	0.199084
C	-1.522484	0.729854	1.094803

W	-0.112183	-0.097839	-0.192821

$^{5}S_{35}$

C	1.507498	1.250300	-0.231072
C	-1.523632	0.730534	1.093002
C	1.464371	-0.949343	0.868980
C	1.971043	0.205410	0.448098
C	-2.036330	-0.038906	0.200805
W	-0.112131	-0.097135	-0.192958

$^{3}S_{36}$

W	0.780366	-0.000114	-0.000026
C	-3.371437	-0.000100	-0.000020
C	-0.889743	0.859029	0.000590
C	-2.235518	0.811129	-0.000435
C	-2.236454	-0.811099	0.000078
C	-0.891358	-0.857551	0.000106

$^{3}S_{37}$

W	-0.470156	-0.067913	0.000020
C	0.630653	1.187931	0.948033
C	1.543177	0.632560	-0.000203
C	2.061572	-0.746395	-0.000064
C	0.933058	-1.423915	0.000161
C	0.630128	1.187410	-0.948174

$^{5}S_{38}$

C	1.832956	-0.747431	0.070774
C	-2.367925	0.000327	-0.262064
C	-1.828229	0.000050	0.906515
C	2.946437	0.000108	0.198414
C	1.832947	0.747656	0.070702
W	-0.195907	-0.000058	-0.079811

$^{3}S_{39}$

W	-0.868154	-0.132862	0.000007
C	3.577961	0.022966	0.000017
C	1.008019	-0.033615	-0.000120
C	4.861112	0.029046	0.000037
C	2.285414	0.014836	-0.000021
C	-1.025275	1.605392	0.000004

$^{1}S_{40}$

C	-0.816435	-1.091423	1.160581
C	2.535523	-0.602602	0.042349
C	0.763543	1.438922	0.542534
C	1.678245	0.492274	0.296117
C	1.333545	-0.783378	-0.551170
W	-0.445494	0.044287	-0.120844

$^{5}S_{41}$

C	-2.150515	0.673515	0.142027
C	1.725170	-0.993063	0.355628
C	-1.733348	-0.334616	0.817081
C	2.031591	0.300468	0.332544
C	1.320656	1.414815	0.192735
W	-0.096775	-0.086037	-0.149190

$^{5}S_{42}$

C	-1.321159	1.414548	0.193237
C	2.151125	0.673117	0.142098
C	1.733364	-0.335065	0.816845
C	-1.724455	-0.993542	0.355288
C	-2.031707	0.299862	0.332541
W	0.096716	-0.085858	-0.149190

$^{3}S_{43}$

C	-1.413730	-0.047682	-0.000077
C	-2.691712	0.171249	0.000193
C	1.770704	1.220804	0.000324
C	0.572394	1.719504	-0.000273
C	-3.969715	0.299562	-0.000016
W	0.464761	-0.272711	-0.000012

$^{5}S_{44}$

C	2.826491	0.507569	0.181493
C	1.787139	-0.137328	0.748671
C	-2.025687	0.271448	0.495425
C	1.726268	0.546939	-0.587515
C	-1.567217	1.374689	0.014763
W	-0.222729	-0.207837	-0.069149

$^{3}S_{45}$

C	1.381023	-0.929957	-0.116064
C	1.642949	0.560057	0.220873
C	-1.047372	-0.494183	1.424909
C	0.706522	1.508799	0.325481
C	2.611968	-0.491975	0.086594
W	-0.429332	-0.012384	-0.157443

$^{3}S_{46}$

C	-2.612171	-0.491796	0.087197
C	-1.642636	0.560186	0.220453
C	-0.706149	1.509016	0.324676
C	1.046685	-0.493411	1.425089
C	-1.381366	-0.929454	-0.116501
W	0.429376	-0.012530	-0.157371

$^{5}S_{47}$

C	0.908643	-1.689424	0.128533

C	0.908573	1.689603	0.128390
C	1.725573	-0.671235	0.236822
C	-1.948262	0.000101	0.743019
C	1.725403	0.671331	0.236934
W	-0.269183	-0.000031	-0.119489

$^{1}S_{48}$

W	0.416726	-0.174942	-0.000019
C	-1.394554	0.124556	-0.818404
C	-1.034899	1.302417	-0.000318
C	-1.790662	-1.017932	-0.000041
C	0.474969	1.624157	0.000248
C	-1.394477	0.124414	0.818752

$^{5}S_{49}$

C	-2.840592	0.218453	0.000350
C	-4.121268	0.457368	-0.000242
C	1.506467	1.326928	-0.000232
C	2.502788	0.523180	0.000445
C	-1.587203	-0.064883	0.000332
W	0.368093	-0.199544	-0.000053

$^{5}S_{50}$

C	1.486299	-0.103825	-0.007213
C	-1.651951	1.176223	0.576426
C	-1.049742	1.628486	-0.473330
C	4.011909	0.441706	0.068942
C	2.733340	0.196672	0.036327
W	-0.448367	-0.270751	-0.016310

$^{1}S_{51}$

C	-1.597546	-0.541748	0.119876
C	-0.636017	-1.190655	0.969617
C	-1.883465	0.887180	-0.264566
C	-0.754346	-1.142928	-0.887315
C	-0.759136	1.416165	0.319107
W	0.456528	0.046377	-0.020815

$^{3}S_{52}$

W	0.449605	-0.132616	-0.000006
C	-1.495665	-0.015010	0.863138
C	-1.495336	-0.014774	-0.863311
C	-1.529454	-1.160507	0.000102
C	0.165611	1.681172	0.000281
C	-1.190280	1.144717	-0.000141

$^{5}S_{53}$

C	-0.947175	0.857825	0.172258
C	-0.946963	-0.857831	0.171895
C	-3.351632	-0.000153	-0.103484

C	-2.272141	0.810679	-0.027945
C	-2.272045	-0.810553	-0.027547
W	0.793780	0.000003	-0.015014

$^{3}S_{54}$

W	0.812109	-0.089919	-0.000139
C	-2.457211	-0.053753	0.745357
C	-0.253397	1.319482	0.002064
C	-2.458056	-0.049702	-0.744128
C	-1.232240	0.249207	-0.000595
C	-3.615106	-0.356231	-0.000988

$^{5}S_{55}$

W	0.427107	0.164685	-0.000032
C	-1.405617	0.846906	0.762709
C	-0.965860	-1.486671	-0.000287
C	-1.722524	-0.307743	-0.000386
C	0.232776	-1.932095	0.000063
C	-1.406431	0.848491	-0.761707

$^{1}S_{56}$

C	1.353913	0.951786	0.649286
C	-1.595514	-0.190450	0.572131
C	1.188339	1.913485	-0.213809
C	-1.325770	0.852700	-0.396815
C	-2.618265	0.656562	0.031386
W	0.243024	-0.339250	-0.052069

$^{3}S_{57}$

C	-0.918077	-1.138365	-0.000081
C	-1.473612	0.350071	0.802820
C	-1.473969	0.349536	-0.802258
C	-2.312465	-0.602267	-0.000008
C	-0.839411	1.419401	-0.000509
W	0.568989	-0.030679	0.000003

$^{5}S_{58}$

C	-1.063845	-1.034337	0.790563
C	-1.380461	1.125570	-0.000262
C	-1.962505	-0.172701	0.000152
C	-0.339960	1.864061	0.000181
C	-1.064070	-1.034431	-0.790467
W	0.471149	-0.060662	-0.000013

$^{5}S_{59}$

W	0.653858	-0.106239	0.000040
C	-3.536482	-0.309468	0.000417
C	-2.150300	-0.129712	-0.000205
C	-0.136895	1.699403	-0.000048
C	-1.005303	-0.965953	-0.000456

C	-1.235265	1.016014	-0.000201

$^{3}S_{60}$

C	1.195112	-0.370502	1.100021
C	1.467759	0.736656	0.195273
C	2.412241	-0.145334	-0.532168
C	0.283324	1.555590	-0.105701
C	1.270641	-0.931017	-0.354485
W	-0.537493	-0.068545	-0.024563

$^{3}S_{61}$

C	-2.412150	-0.145195	-0.531909
C	-0.283149	1.555615	-0.105578
C	-1.270611	-0.930915	-0.354709
C	-1.194836	-0.370867	1.099814
C	-1.467730	0.736757	0.195344
W	0.537444	-0.068546	-0.024565

$^{1}S_{62}$

C	-2.363309	-0.056182	-0.000243
C	-0.083091	1.637855	-0.000850
C	-1.172204	-0.688203	-0.822010
C	-1.171569	-0.685647	0.823044
C	-1.295681	0.840706	-0.000009
W	0.493448	-0.085016	0.000005

$^{3}S_{63}$

C	2.403157	-0.095030	-0.001528
C	1.215586	-0.718665	-0.768013
C	1.336827	0.857892	-0.000701
C	1.218192	-0.717009	0.770027
C	0.194426	1.654512	0.000372
W	-0.516340	-0.079597	-0.000013

$^{5}S_{64}$

C	1.056717	1.609678	-0.000862
C	-4.908365	0.030963	-0.005498
C	-1.055262	-0.018407	0.022030
C	-3.624153	0.026665	-0.009145
C	-2.317976	0.006669	0.009454
W	0.879652	-0.134235	-0.001296

$^{5}S_{65}$

C	2.049891	-0.058363	-0.579031
C	1.328442	-0.353277	0.936441
C	1.354885	0.965546	0.232674
C	0.237763	1.692608	-0.176565
C	1.333560	-1.230563	-0.293649
W	-0.511179	-0.082374	-0.009719

$^{3}S_{66}$

C	0.733508	1.433148	0.714908
C	-2.857364	0.492186	-0.538826
C	-1.115453	-0.708615	0.790708
C	-2.356063	-0.288700	0.554830
C	-1.462545	0.287212	-0.489464
W	0.572264	-0.098532	-0.083688

$^{5}S_{67}$

C	-1.951060	0.142726	0.906195
C	2.713186	-0.330872	0.314589
C	1.647958	0.641812	0.103984
C	0.660041	1.541675	-0.052453
C	1.508416	-0.872398	0.162496
W	-0.371233	-0.091049	-0.116336

$^{3}S_{68}$

C	-1.769535	-0.721138	-0.618808
C	-1.753728	-0.708788	0.645717
C	1.753518	-0.709441	0.645650
C	0.001103	1.936082	0.014328
C	1.768939	-0.722013	-0.618883
W	-0.000024	0.075024	-0.005514

Cartesian coordinates for the global minima, reoptimized using the B3LYP/def2-TZVP model chemistry

----------WC_2----------

$^{5}S_{1}$

C	0.650741	-1.625649	0.000000
C	-0.650741	-1.625358	0.000000
W	0.000000	0.263595	0.000000

----------WC_3----------

$^{3}S_{1}$

C	1.164350	-1.222960	-0.000297
C	1.696819	-0.000084	0.000438
C	1.164633	1.222843	-0.000297
W	-0.326416	0.000016	0.000013

----------WC_4----------

$^{3}S_{1}$

C	-1.524596	0.680806	-0.000093
C	-0.726191	1.760257	-0.000288
C	-0.729868	-1.758823	-0.000282
C	-1.525972	-0.677719	-0.000110

W	0.365402	-0.000367	0.000063

----------WC_5----------

$^3S_1$

C	-1.167486	1.313611	0.129692
C	-1.841114	0.262504	0.498274
C	1.164019	1.316376	0.129953
C	1.840258	0.266698	0.498205
C	-0.002087	1.732045	-0.518297
W	0.000520	-0.396587	-0.059824

Cartesian coordinates for the first 2 most stable WC_2 structures (quintuplet and triplet) reoptimized at CCSD/def2-TZVP level of theory

----------WC_2----------

$^5S_1$

C	0.653082	-1.632849	0.000000
C	-0.653082	-1.632849	0.000000
W	0.000000	0.264786	0.000000

----------WC_2----------

$^3S_1$

C	0.720582	-1.479293	0.000000
C	-0.720582	-1.479290	0.000000
W	0.000000	0.239885	0.000000